

WAVE PROPAGATION IN TWO-DIMENSIONAL PHONONIC CRYSTAL PLATE

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The studies of propagation elastic waves into composite materials have become considerably more frequent in the last years, especially for the composite materials called phononic crystals (PhnCs), which show recurrent variations of the elastic constants and density. The field of PhnCs is only about 10 years old and the search for the best phononic structure is still ongoing. Phononic crystals will provide new components in acoustics and ultrasonic fields, offering functionalities and level of control comparable to the light field. The sizes of the crystals are directly proportional with the wave length, therefore making it possible to create crystals which vary from macro meters to nanometers and frequencies which vary from Hz to THz. Considering the dimensionality rule, these materials can be used in manufacturing from phonic isolating systems to filters, multiplexers or sensors. This study is focused on opening the banned frequency bands into a phononic 2D material through theoretical and numerical studies on surface elastic waves emission. We expose the first results of the numerical simulation conducted on dispersion curves for a PhnCs structure, obtained using the plane-wave expansion method (PWE).

Key words: Phononic crystal, Plane-wave expansion method, Phononic band gaps.

1. INTRODUCTION

The study of elastic/acoustic wave's propagation in periodic structures has originated many novel discoveries in physics in the past decade. Analogies from such subfields in physics have also opened new fruitful avenues in the research on the propagations of classical waves in periodic structures. As an example, the "phononic crystals" (PhnCs) which is composed of artificial periodic elastic/acoustic structures that exhibit so-called "phononic band gap" (PBG), has received a great deal of attention [1–4,7–17] by analogy with the electronic or photonic band gap in natural or artificial crystals. Phononic crystals are similar to photonic crystals but for the peculiarities of elastic as compared to optical waves. These can be created by a one-dimensional, two-dimensional or three-dimensional periodic arrangement of inclusions in a host matrix (Figure 1).

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Several theoretical methods have been used to study the elastic/acoustic structures, such as, the transfer-matrix (TM) method [5], the multiple scattering theory (MST) [7–11], the plane-wave expansion method (PWE) [12–14], the finite difference time domain method (FDTD) [15–17], and finite element method (FEM) [18]. In refs. 7-11, the MST theory was applied to study the band gaps of three dimensional periodic acoustic composites and the band structure of a phononic crystal consisting of complex and frequency-dependent Lamè coefficients. García-Pablos used the FDTD method to interpret the experimental

data of two-dimensional systems consisting of cylinders of fluids Hg, air, and oil inserted periodically in a finite slab of Al host. FEM is one such method which solves the partial differential equations numerically by subdividing the whole domain into finer meshes called elements. Finite element method is a powerful technique to solve partial derivation equations and has long been used by engineers to solve mechanical, structural and electrical problems. There exists a lot of literature on usage of FEM to model acoustic wave devices, but many of them are limited to bulk wave type [18]. Kushwaha utilized the PWE method to calculate the first full band structure of the transverse polarization mode for periodic elastic composites. Surface waves propagating at the surface of a two-dimensional Al-Hg phononic crystal have been observed for first time by Torres et al. [19].

This work is to investigate theoretically and numerically the characteristics of the surface elastic/acoustic waves and plane elastic waves in 2D periodic anisotropic structures based on the PWE method. In the theoretical study we consider 2D phononic crystal with general anisotropy and square lattice in Brillouin zone, where the host material, the circular cylinders of radius r_0 are embedded periodically in background in a solid matrix with lattice spacing a (Figure 2). We choose the $(x-y)$ plane as the plane of the waves guide and z is parallel to the cylinder. All the elastic parameters are independent of z because the 2D phononic medium is invariant in that direction. After this, the symmetry of materials is lowered to trigonal and isotropic for the first numerical results obtained with Matlab program.



Figure 1. Schematic description of a periodic phononic crystal: one, two and three dimensions of the typical structure.

2. PLANE WAVE EXPANSION IN PLANE STRUCTURE

In the first subsection are essentially a summary of the PWE method originally exposed in Ref. [5] in the context of general anisotropy in materials. Subsection II.2 are extensions of the theory to the representation of air holes in a phononic crystal and to the problem of identifying plane modes, respectively. Consider a phononic crystal composed of a two dimensional periodic array ($x-y$ plane) of material **A** embedded in a background material **B** (Figure 2). Both materials are supposed to be homogenous and continuous with the highest symmetry, i.e., belonging to the triclinic symmetry.

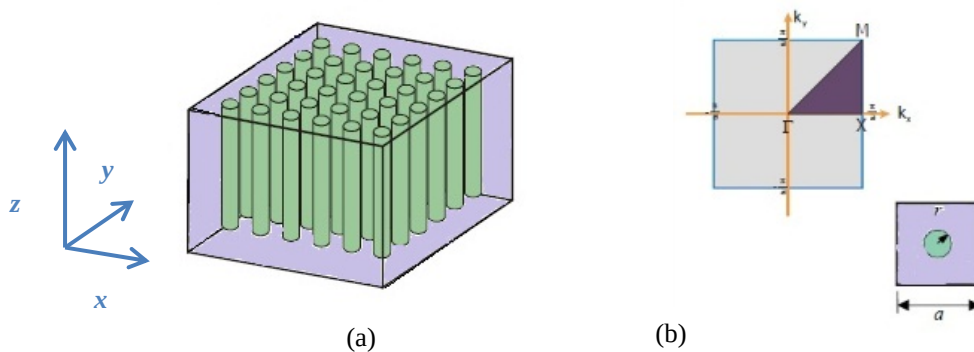


Figure 2. (a) Square-lattice for 2D PhnCs with of cylindrical holes in solid matrix; (b) First irreducible Brillouin zone corresponding of this periodical structure.

2.2. PWE BASICS METHOD

In an elastic solid medium, the mechanical properties of the material used to connect the stress to deformation by a law called the law of behavior. 1'hypothèse in small strain, this relationship is linear:

$$\sigma_{ij} = C_{ijkl} S_{kl} \quad (1)$$

where $i, j, k, l = \overline{1,3}$, C_{ijkl} is the elastic stiffness tensor and S_{kl} is the strain-displacement.

The strain tensor is defined in relation to movement u :

$$S_{kl} = \frac{1}{2} \left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \quad (2)$$

Substituting Eq. (2) into Eq. (1), we obtain the law of Hooke

$$\sigma_{ij} = C_{ijkl} \frac{1}{2} \left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \quad (3)$$

Voigt notation is the standard mapping for tensor indices and coupling indices ij and kl as follows:

i	j
1	xx
2	yy
3	zz
4	yz,zy
5	xz,zx
6	xy,yx

It is then possible to use contracted notation and Hooke's law is written:

$$\sigma_{\alpha\beta} = C_{\alpha\beta} S_{\beta} \quad (4)$$

where $\alpha, \beta = \overline{1,6}$. The elasticity matrix $C_{\alpha\beta}$, with its 21 elasticity coefficients, represents the most general case of crystal system triclinic symmetry. This matrix takes the form:

$$C_{\alpha\beta} = \begin{pmatrix} C_{11} & \dots & C_{16} \\ \vdots & \ddots & \vdots \\ C_{61} & \dots & C_{66} \end{pmatrix} \quad (5)$$

In the quasistatic approximation, the forces of gravity and inertia within the solid medium are *neglected*, the fundamental principle of dynamics applied to a solid particle is written:

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} = C_{ijkl} \frac{\partial^2 u_l}{\partial x_j \partial x_k} \quad (6)$$

where $i, j, k, l = \overline{1,3}$ and the position vector will be note $\mathbf{r} = (x, y, z) = (\mathbf{x}, z)$, ρ is the mass density.

Due to the spatial periodicity of the phononic structure (Figure 2), the material constants $\rho(\mathbf{r})$, $C_{ijkl}(\mathbf{r})$ can be expanded in the Fourier series with respect to the two-dimensional reciprocal lattice vectors (RLV), where $\mathbf{G} = (G_1, G_2)$ is the 2D reciprocal vector:

$$\rho(\mathbf{r}) = \sum_{\mathbf{G}} \exp[i(\mathbf{K} + \mathbf{G})\mathbf{x} - \mathbf{G}z] \rho_{\mathbf{G}} \quad (7)$$

$$C_{\alpha\beta}(\mathbf{r}) = \sum_{\mathbf{G}} \exp[i(\mathbf{K} + \mathbf{G})\mathbf{x} - \mathbf{G}z] C_{\alpha\beta}^{\mathbf{G}} \quad (8)$$

$$\mathbf{K} = (K_x, K_y) = (K_1, K_2) \quad (9)$$

is the Bloch wave vector and the frequency

$$\omega = 2\pi f = 2\pi \frac{v}{\lambda} = vK \quad (10)$$

The components of the displacement vector can be written as:

$$u(\mathbf{r}, t) = A_i \exp[i(\mathbf{K} n_k x_k - \omega t)] \quad (11)$$

used the Bloch theorem it rewrites:

$$u(\mathbf{r}, t) = \sum_{j=1}^3 A_j \exp[i(\mathbf{K} + \mathbf{G}_j)\mathbf{x} - \omega t] \exp(iK_z z) \quad (12)$$

The wave propagation is chosen independent of the direction z . The components of displacements on the directions $\mathbf{x}$ (u_1 and u_2) are decoupled from (u_3). So, there is a decoupling of transverse vertical (TV), which are polarized along the direction z from other waves, called longitudinal waves (L) and horizontal shear waves (TH), where the speeds of this waves are: $v_L \gg v_{TH}, v_{TV}$.

2.2 BOUNDARY CONDITIONS AND PROPAGATING MODES

For Lamb modes propagating in a plate structure ($h/2 < z < h/2$, h is the plate thickness), all solutions are kept, i.e. a set of $6n$ partial waves. The displacement vectors can be expressed as:

$$\begin{aligned} u(r, t) &= \sum_g \exp[i(K + G_j)x - i\omega t] \left(\sum_{i=1}^{3n} A_g \exp(ik_z^i z) \right) \\ &= \sum_{j=1}^{3n} \exp[i(K + G_j)x - i\omega t] \sum_{i=1}^{3n} X_i e_i^j \exp(ik_z^i z) \end{aligned} \quad (13)$$

where e_i^j is the associated eigenvector of the eigenvalue k_z^i . The prime of the summation denotes that the sum over is truncated up to n . X_i is the undetermined weighting coefficient which can be determined from the traction free boundary conditions on the surface $z=0$,

$$\sigma_{iz}/z = 0 = C_{izmn} \partial_n u_m / z = \pm h/2 = 0 \quad i = \overline{1,3} \quad (14)$$

Substituting Eq. (13) into Eq. (14), we have:

$$\begin{bmatrix} M_{1,0}^{(1)} & M_{1,0}^{(2)} & \dots & M_{1,0}^{(3n)} \\ M_{2,0}^{(1)} & M_{2,0}^{(2)} & \dots & M_{2,0}^{(3n)} \\ M_{3,0}^{(1)} & M_{3,0}^{(2)} & \dots & M_{3,0}^{(3n)} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_{3n} \end{bmatrix} \equiv \tilde{M}X = 0 \quad (15)$$

$\tilde{M}$ is a $3n \times 3n$ matrix and its components are:

$$M_{1,0}^{(i)} = (C_{\alpha-\alpha'}^{33} + C_{\alpha-\alpha'}^{43} + C_{\alpha-\alpha'}^{53}) [(k_1 + G_1') e_{\alpha}^{3(i)} + k_z^{(i)} e_{\alpha}^{2(i)}] \quad (16)$$

$$M_{2,0}^{(i)} = (C_{\alpha-\alpha'}^{34} + C_{\alpha-\alpha'}^{44} + C_{\alpha-\alpha'}^{54}) [(k_2 + G_2') e_{\alpha}^{3(i)} + k_z^{(i)} e_{\alpha}^{2(i)}] \quad (17)$$

$$\begin{aligned} M_{3,0}^{(i)} &= (C_{\alpha-\alpha'}^{31} + C_{\alpha-\alpha'}^{41} + C_{\alpha-\alpha'}^{51}) [(k_1 + G_1') e_{\alpha}^{3(i)}] + (C_{\alpha-\alpha'}^{32} + C_{\alpha-\alpha'}^{42} + C_{\alpha-\alpha'}^{52}) [(k_2 + G_2') e_{\alpha}^{3(i)}] + (C_{\alpha-\alpha'}^{33} + C_{\alpha-\alpha'}^{43} + \\ &C_{\alpha-\alpha'}^{53}) [k_z^{(i)} e_{\alpha}^{3(i)}] + (C_{\alpha-\alpha'}^{36} + C_{\alpha-\alpha'}^{46} + C_{\alpha-\alpha'}^{56}) [k_1 + G_1' e_{\alpha}^{3(i)} + k_2 + G_2' e_{\alpha}^{3(i)}] \end{aligned} \quad (18)$$

For the existence of a nontrivial solution of X_i , the following condition must be satisfied, i.e.

$$\det(\tilde{M}) = 0 \quad (19)$$

Equation (19) is the dispersion relation for surface waves propagating in two-dimensional phononic crystals with both the filling material and the background material belong to the triclinic system. In this work, we are considered the phononic structures with square lattice. In figure XX are the Brillouin region of the square lattice where the reciprocal lattice vector G is

$$G = \left(\frac{2\pi N_1}{a}, \frac{2\pi N_2}{a} \right) \quad (20)$$

$N_1, N_2 = 0, \pm 1, \pm 2, \dots$ and the filling fraction is $f = \frac{\pi r_0^2}{a^2}$.

RESULTS

The dispersion relations in 2D PhnCs for plate wave's propagation (Eq. 19) are solved by the program MATLAB. The program is designed for modeling engineering problems described by partial differential equations and it is possible to combine different physical models and solve physics problems. To validate the numerical model developed, we chose for the first time, a structure one-dimensional with silicon isotropic material, where the physical characteristics are summarized in Table 1 and the dispersion curves are presented in Figure 3. The band gap in the structure chosen as model is located near the frequency 1.4 MHz and the results are valid with the literature [20].

Material	Symmetry	Density (kg/m ³)	Elastic constants (x10 N/m ²)				
			C ₁₁	C ₁₂	C ₄₄		
Si	isotropic	2331	16.57	6.39	7.962		
			C ₁₁	C ₁₂	C ₁₃	C ₁₄	C ₃₃
LiNbO ₃	trigonal	4650	20.30	5.73	7.52	0.85	24.24
			C ₄₄	C ₆₆			
			5.95	0.72			

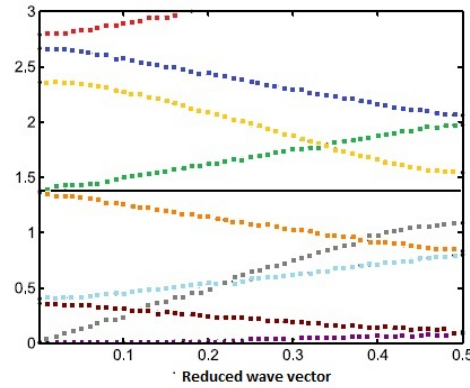
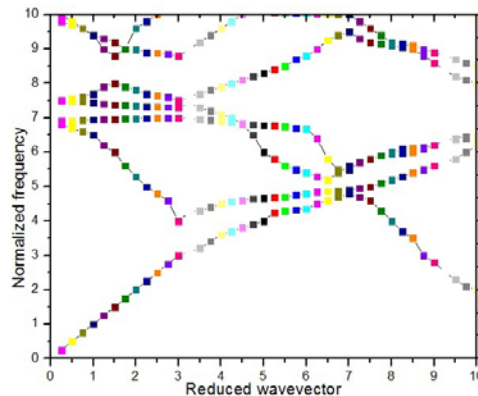
Table 1. The elastic proprieties of Si and LiNbO₃.

Figure 3. Dispersion curves of Lamb wave modes for the 1D two-component composite plate with unit cell area 0.2, length 0.1 mm, height 0.02 mm and lattice parameter 2 mm. The shaded region represents the first band gap of Lamb waves. On abscissa is frequency in MHz.

In general, we follow the realization a SAW devices with phononic crystals in the active zone, so we are interested to study the frequency band gaps in piezoelectric materials like as PZT, LiNbO₃ or quartz. In this work, we are not discussed the piezoelectric proprieties and we are focusing to develop the computer algorithm only for PhnCs with high anisotropy. Still, we exemplify the theoretical theory PWE in the case of trigonal symmetry for lithium - niobate with the square- phononic structure where the wave's propagation in the plane of the surface are along the plan (x-y).

In Figures 4 and 5, the dispersion curves of elastic waves for two structures PhnCs with different filling ratios are plotted. Holes in the structure have a diameter of 412 nm (a), respectively 654 nm (b). We observed an increase in the frequency band gap with increasing filling ratio of the structure. For a report of 64% was obtained the frequency band gap until 180 MHz and 270 MHz (Figure 3, b).

In future simulations we will watch for the different geometry of PhnCs, filling factor, to obtain an optimal structure with frequency band gap as high, close to GHz, specify the type of LiNbO₃ and useful in designing the GHz-SAW devices.

Figure 4. Dispersion curves for square lattice air holes/LiNbO₃ PhnCs with filling factor 49%

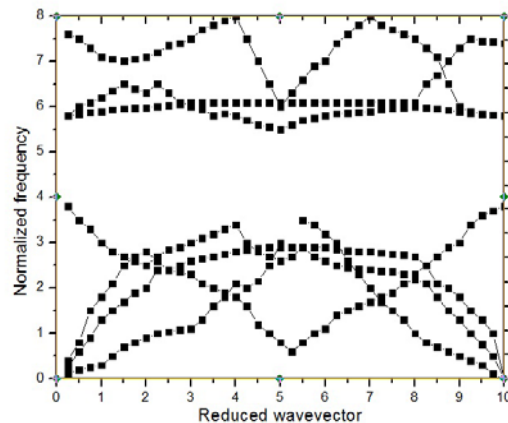


Figure 5. Dispersion curves for square lattice air holes/LiNbO₃ PhnCs with filling factor 64%.

CONCLUSIONS

In this work, a plane wave expansion method suited to the analysis of acoustic wave propagation in phononic crystals has been described for two-dimensional phononic crystal consisting of different materials with general anisotropy. This model brings crowns synthesis of various results so far in the specialty literature by various authors.

Our contribution comes in theoretical model for obtained the surface modes of a square lattice PhnCs made of trigonal structure of lithium niobate material with air circular inclusions. A band gap for surface waves with a filling factor 64% has been found and will continue to optimize the model calculations.

This analytical study is a first stage of our further investigations to obtain SAW devices with PhnCs materials. In the future work we do make theoretical model for a piezoelectric material PhnCs structure to optimize the geometry of the structure for high-frequency band gap, up to several GHz.

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